Use of Surface Soil Moisture to Estimate Profile Water Storage by Polynomial Regression and Artificial Neural Networks

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ABSTRACT

Water storage in the soil profile is an important agronomic variable but its measuring is rather difficult for farmers in production fields. We tested the possibility of using samples from the upper soil layers, which are usually taken for soil fertility evaluation, for whole profile water storage estimation. A data set of 712 water profiles from the subhumid-semiarid portion of the Pampas in Argentina was used, generated under a wide range of soil types, crops, tillage systems, soil cover, and rainfall scenarios. To calculate stored water, soil was sampled up to 140 cm in layers of 20 cm, water content was gravimetrically determined and bulk density also assessed. Polynomial regression and artificial neural networks were used for modeling, randomly partitioning the data set into 75% for model fit and 25% for independent testing. It was possible to estimate with good fit soil profile water storage using as independent variables in regression, or inputs in neural networks, water content in the upper three soil layers (0–20, 20–40, and 40–60 cm) and depth to petrocalcic layer in soils which have this type of horizon. Similar performance was attained with both modeling methods (R^2 > 0.93, RMSE = 11% of mean water content). Other soil and environmental properties had only a minor impact on estimations and were dropped from models. Because of its simplicity, regression is the recommend method for estimation of water content in the soil profile for agronomist.

For many agricultural purposes the determination of soil water storage is a key factor. It controls water availability to crops and yields, influences the partition of rainfall into runoff and infiltration, affecting erosion and flooding, and allows irrigation scheduling. The root zone water status may be measured in the field or estimated by remote sensing and computation modeling. Most common field measurement methods include gravimetric sampling, time domain reflectometry, and neutron gauges (Gardner, 1986; Roth et al., 1990). The former is a direct and simple method that can be used both for research or agronomic goals, but it is rather laborious and time consuming, especially when deep soil layers must be sampled. Time domain reflectometry and neutron gauges require special equipments and calibration against the gravimetric method and are used mainly for research purposes. Additionally, neutron gauges involve biological hazard. When estimation of soil water storage must be performed at middle (catchment) to large (regional) areal scales, remote sensing estimation of surface (5–10 cm) soil water content (Grote et al., 2003) and the assimilation of these data into different types of models for root zone water prediction is the best option (Kostov and Jackson, 1993; Li and Islam, 1999). These methods are suitable for research purposes but not for agronomists and they need validation against field data.

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To overcome the problem of deep sampling, simple linear regression has been used for profile water storage estimation using surface moisture as an independent variable, but this method has usually low prediction potential (Jackson, 1986; Kostov and Jackson, 1993). More powerful empirical modeling options, like polynomial regression (Colwell, 1994; Neter et al., 1990) or artificial neural networks (Joergensen and Bendoricchio, 2001; Özesmi et al., 2006), have not been tested for profile water storage prediction.

The Argentinean Pampas covers approximately 50 Mha (Hall et al., 1992) and because of its extension and yield potential it is considered as one of the most suitable areas for grain crop production in the World (Satorre and Slafer, 1999). Around 50% of the area is cropped under semiarid to subhumid conditions (500–800 mm annual rainfall, Hall et al., 1992). In this portion of the region, soil water storage up to 140 cm is a main controlling factor of crop yields and models have already been developed for yield forecasting including this factor (Bono et al., 2011), but because of the difficulties in sampling, these are not applied by decision makers. Fertilization has become a common practice in the region and soils are generally sampled to 60- cm depth for N evaluation (Alvarez, 2007). We tested the possibility of estimating profile water storage using samples taken from the upper soil layers by two modeling approaches: polynomial regression and neural networks, to develop tools that may allow the prediction of the water storage in the soil profile without the need for additional sampling other than the typical routine sampling for soil fertility evaluation.

MATERIALS AND METHODS

During the 2000 to 2007 period, 149 field experiments were performed in the Semiarid-Subhumid Pampa, widespread across an area of approximately 15 Mha, over a wide range of climate, management, and soil conditions (Tables 1 and 2). A control treatment and different fertilized treatments were compared in each experiment, with two to three replications

Table 1. Soil types, tillage systems, and sampling time of the experiments conducted in the Semiarid- Subhumid Pampa between 2000 and 2007.

Soil type	Experiments	Water profiles	Petrocalcic horizon		Tillage system		Sampling time		
			Yes	No	Tilled	No-till	No living crop	Summer crops	Winter crops
Haplustoll	97	495	294	201	327	168	261	90	144
Hapludoll	43	150	146	4	32	118	76	57	17
Torripsament	3	33	33	0	0	33	20	13	0
Ustipsament	5	19	19	0	16	3	10	9	0
Argiudoll	1	15	0	15	0	15	9	6	0
Total	149	712	492	220	375	337	376	175	161

Table 2. Some properties of the sites sampled in the Semiarid-Subhumid Pampa between 2000 and 2007.

Variable	Minimum	Mean	Maximum
Sampling depth, cm	60	125	140
Clay 0–20 cm, %	2.0	11.2	30.8
Silt 0–20 cm, %	3.6	30.0	51.3
Sand 0–20 cm, %	20.2	58.8	87.5
Organic matter 0–20 cm, %	0.43	1.89	5.69
Water content 0–140 cm, mm	39	238	522
Rainfall from 1 d before sampling, mm	0	2.1	57
Ranfall from 5 d before sampling, mm	0	9	132
Rainfall from 15 d before sampling, mm	0	29.7	234

by nutrient rate (N, P, S, and combinations) in randomized block designs. The most common summer crop was sunflower (*Helianthus annuus* L.) (80%) and the most common winter crop was wheat (80%). The agricultural phase of rotations at the experimental sites was usually compounded by sunflower, corn (*Zea mays* L.), and wheat (*Triticum aestivum* L.) in different proportions. Soil was classified at each site according to Soil Taxonomy (USDA, 2003) by describing the profile using an observation pit. Samples were taken from the four walls of the pit for bulk density determination by the cylinder method (Blake and Hartge, 1986). During the fallow period, the crop growing period (vegetative and flowering stages) and after harvest, soil samples were taken with a hand corer in layers of 20 cm up to 140-cm depth, or to the top limit of a petrocalcic horizon, if it appeared within the upper 140 cm of the profile. The corer extracted an approximate volume of 400 cm^3. Three samples were taken from each control plot and some fertilized plots and composited. In surface samples (0–20 cm) texture (Gee and Bauder, 1986) and organic matter (Nelson and Sommers, 1996) were determined, and in all samples, gravimetric water content was assessed (Gardner, 1986). As usually no significant differences were detected in water content between fertilization treatments (ANOVA, $P = 0.05$), they were averaged by experiment, generating 712 soil water profiles (Table 1).

Gravimetric water was transformed into volumetric water content (mm) using soil bulk density, and cumulative water storage in the profile was calculated. In a first step, simple linear regression and correlation methods were used for data analysis (Neter et al., 1990). Polynomial regression and artificial neural networks were tested as modeling techniques for profile water storage estimation. The regression model was a second grade polynomial which incorporated linear, quadratic, and interaction terms (Alvarez and Steinbach, 2011; Colwell, 1994). Soil water storage to 140-cm depth was the dependent variable; climate, soil, and management variables the predictors (rainfall, texture, organic matter, gravimetric water content of surface soil layers and crop or tillage systems as categorical variables). The data set was randomly partitioned into 75% for training and 25% for independent testing of fitted models. Variable selection was performed by forward stepwise and terms were maintained in the regressions if they were significant at $P = 0.05$ by the F test and impacted the R^2 in at least 0.5%. Multicollinearity was checked by the variance inflator factor (Neter et al., 1990). Neural networks were fitted by a supervised learning procedure using the back propagation algorithm for weights fitting (Rogers and Dowla, 1994). Linear transfer functions were used for connecting the input layer with the hidden layer and the output layer with the network output, meanwhile the sigmoid function (Lee et al., 2003) was used for connecting the hidden layer with the output layer. Inputs were scaled by minimax (Somaratne et al., 2005) and network outputs de-scaled to original units. The same independent variables tested for regression analysis were initially tested as neural inputs, implementing a hierarchical approach for variable selection (Schaap et al., 1998). Sensitivity analysis allowed weighting the effect of different inputs on soil water storage by calculating a sensitivity ratio (Miao et al., 2006). Only inputs with a sensitivity ratio >1 were included into networks because lower ratios indicate no impact of the output (Miao et al., 2006). Selected variables were then tested as inputs by a stepwise procedure (Gevrey et al., 2003). The learning rate, epoch size, and network architecture were determined by methods previously described (Alvarez and Steinbach, 2011). Maximum simplification of the networks was aimed for without reducing the prediction ability as judged by R^2. To avoid overlearning, cross-validation was implemented (Özesmi et al., 2006), by fitting networks using a training set (50% data) with early stopping of weight adjustments when R^2 becomes greater than for the validation set (25% data) (Park and Vlek, 2002). And independent test of the models was performed with 25% of the data. The data set used for testing networks was the same as that used for testing regressions. Networks were developed with Statistica (www.statsoft.com).

A second group of models was developed by similar statistical procedures than those described above but using an estimation of the volumetric water content of the surface soil layers calculated with the average soil bulk density of each soil layer (0–20 cm: 1.21 g mL^{-1}; 20–40 cm: 1.33 g mL^{-1}; 40–60 cm: 1.31 g mL^{-1}) instead of measured bulk density at each site.

Root mean square error (RMSE) of models were calculated (Kobayashi and Salam, 2000) and contrasted (Alvarez et al., 2011). The determination coefficients of models were also contrasted (Kleinbaum and Kupper, 1979). Intercepts and slopes of

Table 3. Correlation matrix of site variables.

Variable	Organic matter	Sand	Silt	Clay	Water 0–20 cm	Water 20–40	Water 40–60 cm	Water 60–80 cm	Water 80–100 cm	Water 100–120 cm	Water 120–140 cm	Rainfall 15 d	Rainfall 5 d
	%												
Sand, %	−0.624†												
Silt, %	0.542	−0.962											
Clay, %	0.677	−0.895	0.747										
Water content 0–20 cm, mm	0.389	−0.306	0.276	0.321									
Water content 20–40 cm, mm	0.441	−0.413	0.377	0.422	0.896								
Water content 40–60 cm, mm	0.400	−0.400	0.363	0.414	0.778	0.895							
Water content 60–80 cm, mm	0.357	−0.397	0.368	0.397	0.649	0.789	0.925						
Water content 80–100 cm, mm	0.277	−0.337	0.308	0.347	0.555	0.698	0.854	0.953					
Water contet 100–120 cm, mm	0.212	−0.292	0.270	0.298	0.509	0.645	0.801	0.908	0.970				
Water contet 120–140 cm, mm	0.162	−0.213	0.192	0.227	0.485	0.598	0.706	0.814	0.898	0.935			
Rainfall from 15 d before sampling, mm	0.005	0.040	−0.054	−0.005	**0.215**	**0.145**	**0.107**	0.036	0.001	−0.001	0.015		
Rainfall from 5 d before sampling, mm	−0.053	**0.158**	**−0.163**	**−0.117**	**0.224**	**0.105**	0.076	−0.012	−0.040	−0.045	−0.022	**0.457**	
Rainfall from 1 d before sampling, mm	−0.030	0.077	−0.080	−0.052	0.058	0.004	0.059	−0.019	−0.026	−0.047	−0.060	**0.253**	**0.462**

† In bold: correlation coefficients significant at $P = 0.05$.

regressions of observed vs. estimated data were compared against 0 and 1 by the *t* using IRENE (Fila et al., 2003). In all cases P was 0.05.

RESULTS

Gravimetric water content at different depths was significantly correlated and correlation coefficients were higher as closer the soil layers (Table 3). Water content was greater in fine- textured soils and as organic matter increased. A weak association was detected between rainfall and water storage in the upper 60 cm of the profile, but this association disappeared at deeper layers. Poor results were obtained using simple linear regression for predicting profile water storage. If water content in the 0- to 20-, 0- to 40-, or 0- to 60-cm layers were used as predictors of cumulative water storage to 140-cm depth, R^2 were 0.49, 0.57, and 0.65, respectively.

Soil water profile showed four different trends (Fig. 1). In cases in which moisture content was nearly constant with depth, cumulative water storage fitted to linear functions and the slope of the regression depends on the volumetric water content. If surface soil layers were wetter than deep layers a convex function fitted to cumulative water storage and, conversely, when surface layers were drier than deep soil, a concave function adjusts better. A consequence of these trends is that linear regression does not fit well to water data and models that can accommodate to curvilinear tendencies are needed.

Polynomial regression and artificial neural networks made both a good job estimating soil water storage (Fig. 2). The

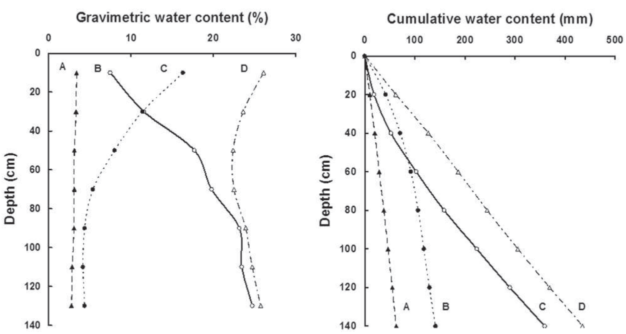

Fig. 1. Examples of soil water profiles taken from the pampean data set. Subfigure in the left shows gravimetric water content of soil layers of 20 cm; subfigure in the right shows cumulative water content. (A) whole soil profile dry, (B) surface layers dry and deep layers wet, (C) surface layers wet and deep layers dry, and (D) whole soil profile wet.

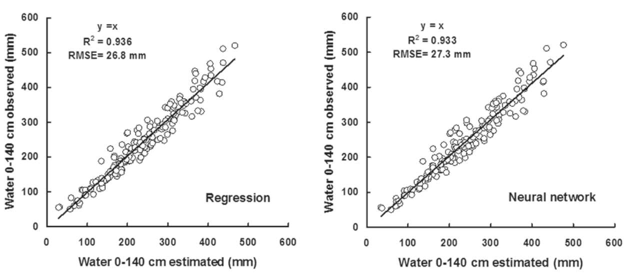

Fig. 2. Observed vs. estimate soil profile water storage (0–140 cm) of the test data set estimated by two methodologists: polynomial regression and artificial neural networks. Estimations were performed using measured soil bulk density for each site. The artificial neural network model may be obtained from the corresponding author on request.

best regression model included as predictors volumetric water content in two soil layers, 0 to 40 and 0 to 60 cm and depth to petrocalcic horizon (Table 4). Other independent variables were dropped from models because of their minimum impact on profile water estimation. The best neural network used as inputs volumetric water content of the 0- to 20-, 20- to 40- and 40- to 60-cm layers and depth to petrocalcic horizon with a 4:5:1 architecture. The generalization capacity of models was high because no significant differences were observed between R^2 and RMSE of training (or training+validation) and test data sets, neither significant difference was detected between the performances of modeling methods. The RMSE were equivalent to approximately 11% of average soil water storage. If models were developed using only volumetric water content in 0- to 20- or 0- to 40-cm depths, the prediction potential decreased (Table 5). Regression models or neural networks could be fitted to water profiles of soils without petrocalcic horizon with similar performances than those obtained for all soils (results not shown).

Models developed using as predictor volumetric water content calculated with average soil bulk density instead of measured density had lower fits than previous models but allowed also a good estimation of profile water storage (Fig. 3, Table 4). No significant differences were detected between the training + validation data sets adjustments of the models and their performance with the test data set, neither significant difference existed between modeling techniques. Root mean square errors rounded 13 to 15% of average profile water storage. Regression model used as predictors volumetric water content in the 0- to 20-, 20- to 40- and 40- to 60-cm layers and depth to petrocalcic horizon and the neural network had the same inputs and architecture that the previous one.

Table 4. Parameters of the polynomial regression modes fitted for soil water storage estimation to 140-cm depth. Model 1 was fitted using measured soil bulk density at each site; model 2 was fitted using average bulk density for the 0- to 20-, 20- to 40-, and 40- to 60-cm soil layers.

Model term	Parameters	
	Model 1	Model 2
Intercept	ns†	ns
D‡	ns	–0.825
D^2	ns	0.00547
$W_{0–20}$	ns	ns
$(W_{0–20})^2$	ns	–0.252
$W_{0–40}$	0.220	1.09
$(W_{0–40})^2$	ns	–0.322
$W_{0–60}$	ns	ns
$(W_{0–60})^2$	–0.0275	–0.101
$D \times W_{0–20}$	ns	ns
$D \times W_{0–40}$	–0.0750	–0.0935
$D \times W_{0–60}$	0.0664	0.0773
$W_{0–20} \times W_{0–40}$	ns	0.447
$W_{0–20} \times W_{0–60}$	ns	–0.112
$W_{0–40} \times W_{0–60}$	0.0395	0.310

† ns = not significant.

‡ D = depth to petrocalcic horizon in soils with this type of layer (cm), otherwise 140). $W_{0–20}$, $W_{0–40}$, and $W_{0–60}$ = soil water content in different soil layers (mm).

Table 5. Performance of two modeling methods for predicting soil profile water storage (0–140 cm) as a function of surface soil moisture in different layers and depth to the petrocalcic horizon.

Variables in model	Regression		Neural network	
	R^2	RMSE	R^2	RMSE
		mm		mm
Depth + water 0–20 cm	0.668	55.7	0.663	55.0
Depth + water 0–40	0.834	42.8	0.824	43.3
Depth + water 0–60 cm	0.936	26.8	0.933	27.3

DISCUSSION

Our results showed that it is not possible to perform a good estimation of profile water content by simple regression using surface soil moisture, even measuring volumetric water content in a broad (0–60 cm) upper soil layer. Only in cases in which variation of water content between soil layers is small, cumulative water profile tends to be linear. Past work has shown similar results. Soil water content of nearby soil layers is highly correlated, but correlation coefficients decrease as layers are more distant (Arya et al., 1983; Kostov and Jackson, 1993), leading to a poor estimation of root zone water storage by regressing on surface moisture (Arya et al., 1983; Jackson, 1986; Jackson et al., 1987; Kostov and Jackson, 1993). Parameters of regression models are site or growing stage specific and cannot be extrapolated to different scenarios than those for which they were adjusted (Jackson, 1986; Kostov and Jackson, 1993). Usually, linear regression estimations are better when soils are at hydraulic equilibrium and there are no water fluxes between layers (Jackson, 1986; Kostov and Jackson, 1993).

The modeling approaches tested here allowed a good estimation of profile water storage because they are suitable techniques for describing curvilinear responses (Batchelor et al., 1997; Colwell, 1994). When feeding polynomial regression or neural networks with moisture measurements from at least two different soil layers they could detect the curvature trend of the cumulative water stored function and predict water storage up to 140-cm depth. The error of the models fitted in this research are greater than those reported in studies that use remote sensing for surface water determination and estimate profile water storage by hydraulic-process based modeling (Galantowicz et al., 1999; Hoeben and Troch, 2000; Wagner et al., 1999), These studies reported RMSE varying usually from 4 to 8% when predicting water stored up to 1-m depth, but the statistical approaches we tested are much more simple and can be applied over a wide set of environmental conditions. They can be used for soil water storage estimation before crop

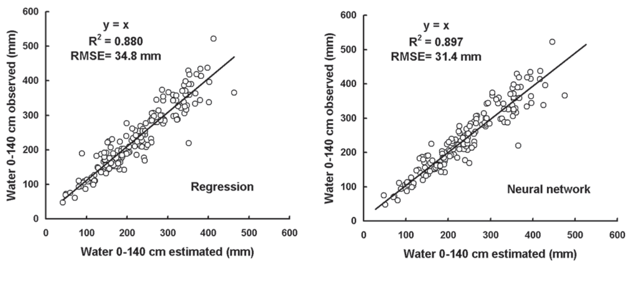

Fig. 3. Observed vs. estimate soil profile water storage (0–140 cm) of the test data set estimated by two methodologists: polynomial regression and artificial neural networks. Estimations were performed using average soil bulk density for the 0- to 20-, 20- to 40- and 40- to 60-cm soil layers. The artificial neural network model may be obtained from the corresponding author on request.

seeding and yield forecasting or also during the growing season for soil moisture studies. When soil bulk density data is available or the soil corer used for sampling allows measurement of bulk density, more precise estimations of water stored in the profile may be attained, but the use of average values of bulk density instead of measured values is possible when calculating volumetric water content of surface layers.

Spatial variability of water storage had been poorly studied in the Pampas. Some work had shown than in soils of the Semiarid-Subhumid Pampa acceptable errors may be attained when water storage is measured at 10 sites within small watersheds (8 ha) (Ferreyra et al., 2002). The common procedure used in the region for sampling destined to fertility evaluation is to sample production fields at around 20 sites (Alvarez, 2007). Consequently, sampling strategies adopted for fertility evaluation purposes are suitable for water storage estimation of small plots. For extended production fields more research is needed to determine sampling density. Because of its simplicity polynomial regression is recommended as a predicting tool for agronomists. The proposed methodology can be used in other regions but validation of the empiric models fitted or new developments are needed.

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